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MORRIS BROWN COLLEGE

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November 11, 1997

Mr. Charles A. Luther
Program Manager/Officer ONR 321
Office of Naval Research
800 North Quincy Street
Arlington, Virginia 22217-5660

Dear Mr. Luther:

It has come to my attention that the Final Technical Report for the program entitled "***Educational Program Improvement In Chemistry Through The Acquisition of GC/MS And FT-NMR Instruments***" (grant number: N00014-95-1-1261) has not been submitted. As required, three copies of the report are enclosed. Additional copies of the report have been sent to the appropriate agencies according to the distribution list.

As indicated in the report, the instruments were installed in May 1996, and we have been using them since that time. Further, as indicated in the report, these instruments have enabled us to broaden the scope of our teaching and learning by providing hands-on experience with state-of-the-art instrumentation for our students. Currently, we are using these instruments routinely in faculty research as well as undergraduate student research. We believe that we are achieving the educational objectives that were defined in the grant request.

The Chemistry Department at Morris Brown College is grateful for the support given by the Office of Naval Research.

Sincerely,

Gloria L. Anderson

Gloria L. Anderson, Ph.D., FAIC, CPC
Principal Investigator
Fuller E. Callaway Professor of Chemistry &
Dean of Science and Technology

"Educational Program Improvement In Chemistry Through The Acquisition of GC/MS And FT-NMR Instruments"

Final Technical Report
Grant Number: N00014-95-1-1261

Submitted
To

Program Manager/Officer ONR 321
Charles A. Luther
Office of Naval Research
800 North Quincy Street
Arlington, Virginia 22217-5660

By

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November 1997

INTRODUCTION

During 1995 the Chemistry Department at Morris Brown College was awarded a grant by the Office of Naval Research (grant number: N00014-95-1-1261), Department of Defense. The purpose of this grant was to enable the department to acquire instrumentation necessary for incorporating the theory and practice of Gas Chromatography/ Mass Spectrometry (GC/MS) and Nuclear Magnetic Resonance (NMR, ^{1}H, ^{13}C, ^{19}F) into laboratory courses. Specifically, the educational objectives of the project were:

1. ***To improve students knowledge of the elementary theory of GC/MS and NMR;***

2. ***To increase students knowledge/skills in the interpretation of GC/MS and NMR spectra;***

3. ***To help students learn the capability of GC/MS and NMR as analytical tools; and***

4. ***To help students learn hands-on operational techniques of GC/MS and NMR instruments.***

To achieve these objectives, we requested a grant from ONR to acquire the necessary GC/MS and FT-NMR instruments. These instruments would enable us to conduct experiments involving the determination of molecular weights and formulas of compounds; the analysis of fragmentation patterns to assist in structure determination; organic qualitative analysis; monitoring product formation during organic reactions; and characterization of potential biologically active compounds. Students would be able to use GC/MS and FT-NMR data to assist in structural determination during the completion of their undergraduate research projects. Faculty would be able to use these instruments in their research, thereby, increasing research productivity.

RESULTS AND DISCUSSION

Acquisition of Instruments

The following instruments were acquired under the ONR grant:

1. ***200 MHz $^{1}H/^{13}C$ GEMINI 2000 High Resolution NMR Spectrometer System [4.7T 54-mm Bore Superconducting Magnet; VNMR Object Code Site Sub-license (1/4 inch tape); WALTZ Modulator ^{1}H-$^{19}F/^{15}N$-^{31}P Switchable Probe, 5 mm, VT, 200 NB; SPARCclassic Computer 644 Mbyte Internal CD-ROM Drive; HP LaserJet IV Printer/Plotter; $135,750]; and***

2. ***GC/MS System (HP 5972A MSD ChemStation System; Chromatographic Mainframe; Mass Selective Bundle; NIST MS ChemStation Library of 74,828 spectra of of 62,235 compounds on 3.5" media; $55,433).***

These instruments were installed in May 1996 and have been operational on a daily basis since that time.

Principle Applications of Instruments

The principle applications for these instruments have been as diagnostic tools in the organic chemistry course as well as undergraduate research. The GC/MS has also been used to provide data for students in the general chemistry laboratory. Hands-on experience in operating the GC/MS instrument has been provided for students in the organic chemistry course and undergraduate research. Because of time requirements, fewer students have had hands-on experience with the FT-NMR spectrometer than with the GC/MS. Most often students are taught to use the instruments during the summer months and on Saturday during the academic year. In general, students are excited about using these instruments, particularly the GC/MS.

Organic Chemistry Laboratory

In the Organic Chemistry Laboratory the GC/MS is used to determine molecular weight of known compounds and to monitor product formation during organic reactions. We plan to add experiments that involve the use of GC/MS to determine structures of simple unknown compounds based upon fragmentation patterns in comparison with spectra stored on file in the data base of the instrument.

The FT-NMR spectrometer is used primarily to obtain spectra for structure determination of simple organic coupounds. We plan to add experiments that require the use of the FT-NMR to provide data essential to identifying reaction products obtained in the laboratory. Additionally, since isotopic labeling is useful as a means of studying reaction mechanisms, we plan to add an experiment that involves the use of FT-NMR to examine a deuterium labeled compound. Deuterium labeled anisole will be prepared by quenching the Grignard reagent (obtained from p-methoxybromobenzene) with D_2O instead of H_2O. The amount of deuterium introduced into the molecule will be determined by ^1H and ^{13}C NMR.

Undergraduate Research

Currently, the primary focus of the principal investigator's research is the development of novel synthetic methods for preparing potential antiviral/antitumor drugs. Specifically, the research involves the synthesis of some 1-substituted and 1,3-disubstituted adamantane derivatives with potential antiviral/antitumor activity.

The GC/MS and FT-NMR instruments are being used extensively by faculty, staff, and students who are conducting research. Presently, the principal investigator has three students enrolled in undergraduate research, four undergraduate research assistants, and one research chemist conducting research in her laboratory. The undergraduate research assistants are enrolled in the organic chemistry course taught by the principal investigator.

The undergraduate research students and their projects are:

1. ***Ms. Cointa Oliver***
   "Potential Antiviral/Antitumor Drugs: The Synthesis and Characterization of Some N-Substituted-1-Adamantyl Acetamides"

2. ***Mr. Ryan Jinks***
   "Potential Antiviral/Antitumor Drugs: The Synthesis and Characterization of Some N-Substituted-1-Adamantane-carboxamides"

3. ***Ms. Emily Cunningham***
   "Potential Antiviral/Antitumor Drugs: The Synthesis and Characterization of Some N-Substituted-1-Adamantylmethyl-amines"

The research chemist is conducting research on ***"Potential Antiviral/Antitumor Drugs: The Synthesis and Characterization of Some Chalcone Like Adamantane Derivatives."*** The undergraduate research assistants are learning synthetic techniques and characterization methods by working under the direct supervision of the research chemist. It is worthy of note that a student who graduated in May 1997, completed his undergraduate research in the principal investigator's laboratory and is now enrolled in a doctoral program at the Georgia Institute of Technology. The title of his study was ***"Potential Antiviral Drugs: The Preparation of N-(1-Adamantyl) N'-Hydroxyurea."***

Prior to the acquisition of these instruments, we had synthesized more than one hundred compounds, many of which had not been fully characterized. Since the acquisition of these instruments, we have synthesized more than fifty additional compounds. These instruments have enabled us to fully characterize previously synthesized compouds as well as those synthesized after the acquisition. They are invaluable tools for monitoring product formation during organic reactions and characterizing reaction products.

Summary

The acquisition of the GC/MS and FT-NMR has enabled us to broaden the scope of our teaching/learning to include techniques that have rapidly become the instrumental techniques of choice of many colleges/universities as well as industry. Exposure to mass spectroscopy and NMR spectroscopy in the laboratory has significantly enhanced our students preparedness to meet the challenges in their future careers, and also has become a vital part of their undergraduate education. Additionally, the acquisition of these instruments has increased our research capability significantly. We believe that we are achieving the educational objectives that were defined in the grant request.

The Chemistry Department at Morris Brown College is grateful to the Office of Naval Research for support of this project.